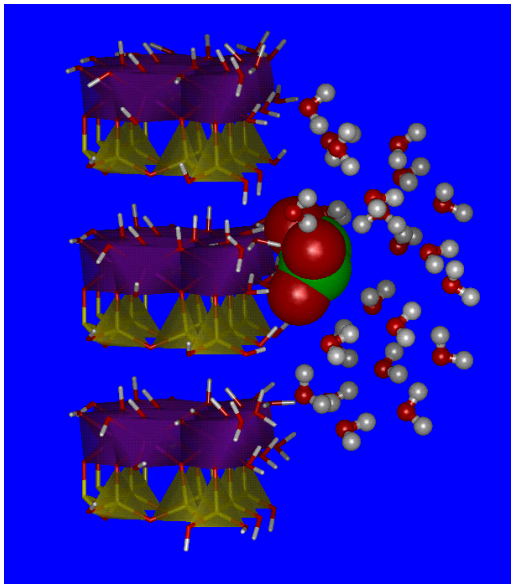
Sandia National Laboratories

Atomistic and Molecular Simulations in Geochemistry and Materials Science

Description

Atomistic and molecular simulations of many geochemical and materials science processes are based on molecular mechanics and quantum-chemical calculations. Empirical methods utilize selected forcefields and can examine static and dynamic interactions of mineralogic and aqueous systems containing up to 5000 atoms when performed on modern workstations. *Ab initio* calculations, however, often require the use of more powerful computers to calculate both chemical reactions and electronic structures, especially for periodic systems. Simulation techniques include:

- Energy Minimizations
- Molecular Dynamics (MD)
- Ionic Modeling
- Monte Carlo
- Hartree Fock Molecular Orbital
- Local Density Functional Molecular Orbital



Sorption of Solvated Oxalate Anion onto (010) Edge Site of Kaolinite Clay

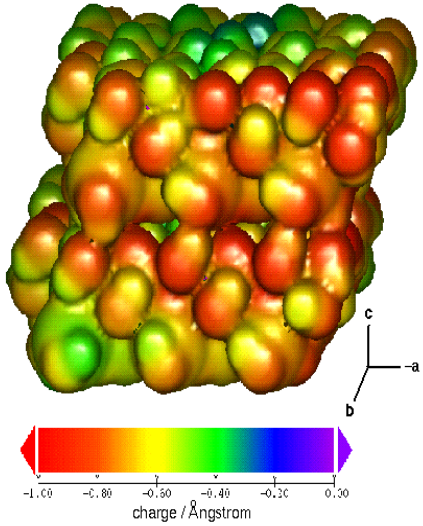
Needs

Geochemistry

- Bulk mineral structure refinement
- Characterization of surface relaxation
- Metal and organic ion sorption mechanisms
- Reactivity of mineral-solution interfaces
- Precipitation and dissolution reactions

Materials Science

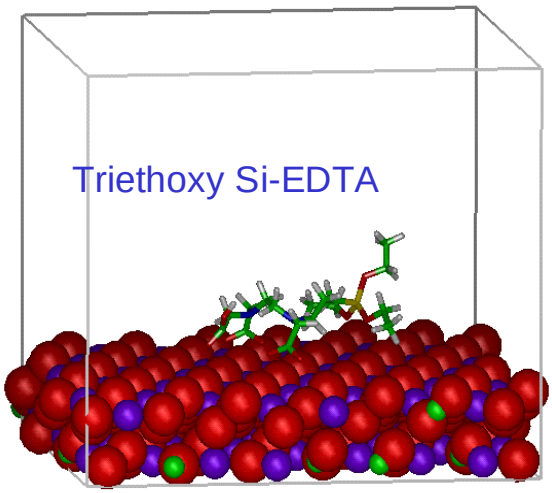
- Sol-gel precursor conformations
- Ionic diffusion rates and mechanisms
- Ceramic growth morphology
- Substrate binding mechanisms



Molecular Electrostatic Potential Surface or (010) Kaolinite Clay

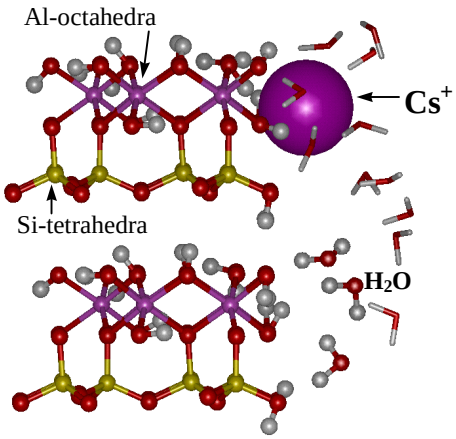
Passivant-Consolidation Coatings

Energy minimizations of sol-gel coatings that best conform to carbonate surface and inhibit reaction



Calcite (104) surface

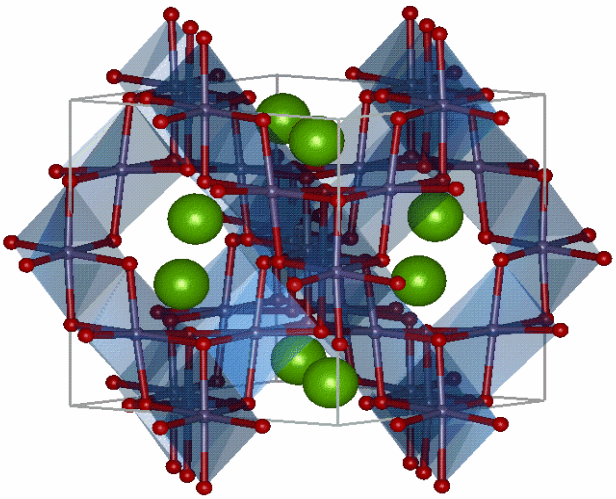
T = 300K
t = 15.6 psec



(010) View

Metal Sorption on Clay Minerals

MD simulation of inner-sphere sorption of CS^+ ion onto aluminol site at (010) edge of kaolinite



Development of Battery Cathode Materials

Energy minimizations and MD studies of metal dopants on bulk structure and Li diffusion

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